NCCS Snapshot
The Week of September 1, 2008

NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES

Oak Ridge National Laboratory
U.S. Department of Energy

Supercomputing Simplified

ADIOS boosts big science

- **An I/O componentization, dubbed ADIOS and developed in part by the NCCS's Scott Klasky, is turning heads with its I/O improvements on codes such as GTC and Chimera**
- **During recent runs on Jaguar the I/O time for a Chimera simulation went from approximately 20 minutes to 1.4 seconds, an improvement of 1,000 times**
- **ADIOS is inserted into an application's XML files, leaving the source code untouched.**
- **Besides I/O, it also allows for real-time visualization and data multiplexing**

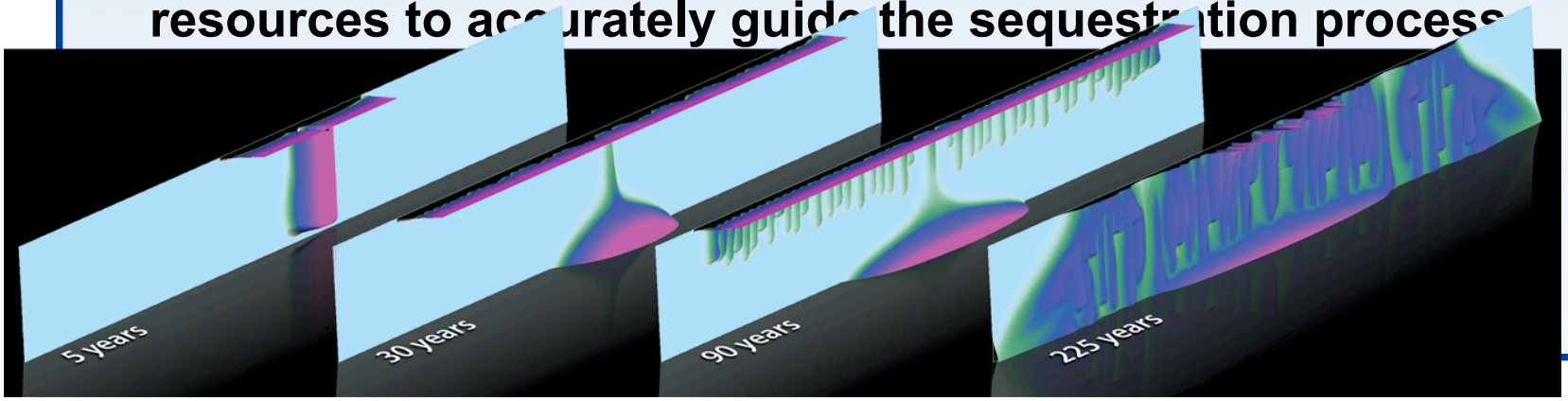
"This huge amount of data needs fast and smooth file writing and reading. With poor I/O, the file writing takes up precious computer time and the parallel file systems on high -performance computing systems can choke."

Fusion researcher and ADIOS user Yong Xiao, University of California-Irvine.

Tap It and Trap It

Groundwater simulation addresses the challenges of carbon sequestration

- **A team led by LANL's Peter Lichtner is using the NCCS's Jaguar to simulate carbon sequestration**
- **The process involves capturing CO_2 from power plants and storing it deep underground, sparing the atmosphere the pollution**
- **With Jaguar the team was able to conduct the largest groundwater simulations ever with an application known as PFLOTRAN**
- **With the era of the petascale, Lichtner anticipates having adequate resources to accurately guide the sequestration process**



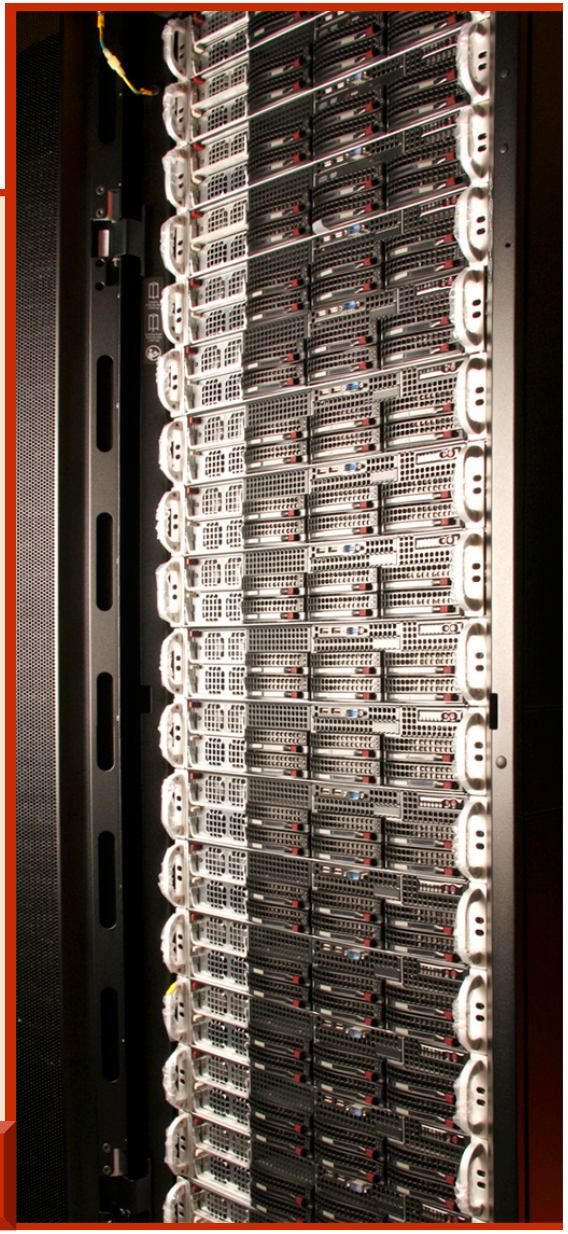
Carbon dioxide dissolving in a deep saline aquifer.

Smoky Stepping Stone to Big Science

- Jaguar may be the NCCS's flagship system, but the big cat gets plenty of big help
- Smoky (named after the UT mascot) was purchased to offload debugging and development from Jaguar to a smaller yet capable system
- Smoky's utility lies in its programming environment which closely mirrors Jaguar
- An 11.7 TF system, Smoky consists of 320 quad-core processors and 2.5 terabytes of memory

"It's the bullpen for science, getting the players ready for the big game. Without Smoky, development would be seriously slowed down, as everyone would have to wait in line on Jaguar."

NCCS staff member Bobby Whitten



System proves its worth in scaling, debugging

Business Liaison Joins ORNL

Tichenor has long experience creating HPC partnerships


Suzy Tichenor

- **Suzy Tichenor, recently of the Washington -based Council on Competitiveness, has joined ORNL's Computing and Computational Sciences Directorate as director of its Industrial Partnership Program.**
- **She will serve as the principal interface between the ORNL organization and industry**
- **Tichenor has more than 20 years experience creating partnerships and programs from within the government, the private sector, and not-for-profit organizations**

"Suzy has a unique understanding of how industry is using high-performance computing to drive innovation and productivity. She will bring tremendous energy and focus to our industrial outreach activities."

Thomas Zacharia, ORNL associate laboratory director for computing and computational sciences